ABSTRACT

        The present invention provides methods for the generation of virtual libraries of compounds. These compounds are generated *in silico*. The present invention encompasses methods for tracking the addition of fragments, use of reagents, and transformations
5   performed. Further, methods for interfacing the information necessary to generate libraries of compounds with instrumentation that conducts the actual synthesis of the compounds are provided. Also provided are methods for the *in silico* docking of the library compounds to identified target molecules of interest.